Chlorotrifluoroethylene 79-38-9 | DTXSID3026485

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Weighted KNN model

5-fold CV (75	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 2170 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.13e-01

Confidence level: 7.01e-01

Nearest Neighbors from the Training Set

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Dichloroacetyl chloride

Measured: 4590 Predicted: 29.7

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tert-Butyl hydroperoxide

Measured: 362 Predicted: 5.98

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1,1,2-Trichloropropane

Measured: 890 Predicted: 8.26

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Trimethylamine Measured: 803 Predicted: 862

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1,2-Difluoro-1,1,2,2tetrachloroethane **Measured:** 2010 **Predicted:** 92.7